Session D: Finite Differences

In this short exercise we introduce the concept of *finite differences*, which we will expand upon in subsequent exercises. Finite differences are an important tool in numerical analysis. numerical methods are needed in problems where there may be no analytic solution. We therefore need a scheme that will allow us to approximate the solution and to express that problem in such a way that it can be solved by a computer.

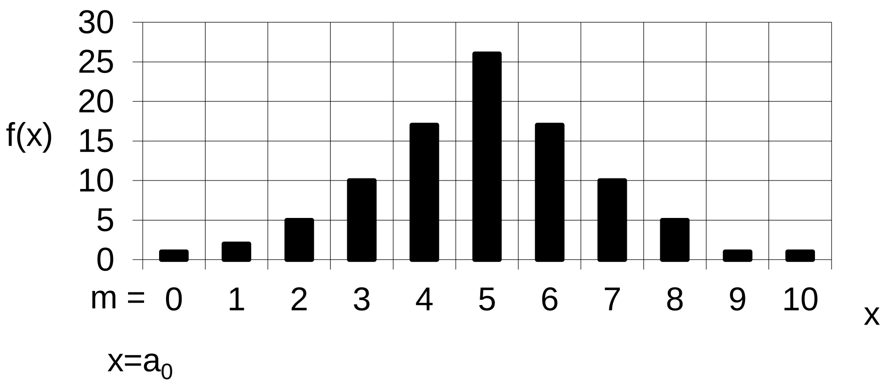
D.1 Introduction

Often we have values of a continuous function, $f(x)$, at discrete values of the variable, x. This can occur if we make measurements at a series of values of x and wish to determine the corresponding function. Finite difference techniques allow us to obtain the maximum amount of information on the underlying continuous function based on these discrete measurements.

Alternatively, we may wish to perform some computation to solve a problem that is expressed in terms of continuous variables (space, time, angle, energy etc.) but that has no simple analytical solution. Finite difference methods allow us to discretise the problem and calculate values of $f(x)$ at a series of specific points, known as *mesh* points. We can then **interpolate** in order to *estimate* the value of the function at intermediate points between the mesh points. We shall look at interpolation later.

D.2 Defining the mesh

Let us first define the nomenclature that we will use while considering finite difference techniques. Consider a series of points measured on a physical x scale:



We label the mesh points where the function is measured as $m = 0, 1, 2, 3, 4$ etc. The first mesh point ($m = 0$) is at $x = a_0$, where a_0 is usually a dimensionful number.

If the spacing of the mesh points is uniform and the distance between mesh points is h, also dimensionful, then the values of x at which mesh points occur are: a_0, $a_0 + h$, $a_0 + 2h$, etc. That is, we have measured values of the underlying physical function $f(x)$ at $f(a_0 + mh)$.

We can write this more succinctly as $f(x_m)$ or $f(m)$ or just f_m.

D.3 Finite Difference Operators

Generally we need to refer to more than one mesh point at a time. For example, we can calculate the local gradient of the underlying function by comparing the values of neighbouring mesh points. We can define a series of finite difference *operators* to help us achieve this.

1.	Forward shift operator	E	$E\{f(m)\} = f(m+1)$
2.	Forward difference operator	Δ	$\Delta\{f(m)\} = f(m+1) - f(m)$
3.	Backward difference operator	∇	$\nabla\{f(m)\} = f(m) - f(m-1)$
4.	Central difference operator	δ	$\delta\{f(m)\} = f(m+\frac{1}{2}) - f(m-\frac{1}{2})$
5.	Averaging operator	μ	$\mu\{f(m)\} = \frac{1}{2}\left[f(m+\frac{1}{2}) + f(m-\frac{1}{2})\right]$
6.	Differential operator	D	$D\{f(m)\} = (\mathrm{d}f/\mathrm{d}x)_m$ i.e. evaluated at $x = a_0 + mh$

Exercise D.1

1. Produce a spreadsheet with a column of values for x running between 0 and 20.
2. Produce a second column for a function of x. For this first case choose $f(x) = x^2$.
3. Now produce columns for E, Δ and ∇.
4. What happens at $m = 20$ for the E and Δ operators and at $m = 0$ for the ∇ operator?
5. Save your spreadsheet to disk.
6. Open it again and now save it under a new name. You thus have two copies.
7. Alter the second copy so that now $f(x) = x^2 + c$ where c is a constant. You can do this by putting c in a blank cell in the spreadsheet and using *absolute* addressing. If you are not sure how to do this, ask a demonstrator.
8. Confirm that the resulting E, Δ and ∇ columns contain what you would expect.
9. Make a new spreadsheet with x values from 0 to 10 but with a blank line between each row of values. Create a separate column for the $f(x)$ values, taking $f(x) = x^2$ as before.
10. Set up columns for values of δ and μ for $m = 0.5, 1.5, \ldots$ etc.

Finite difference operators have the following two properties:

(a) All operators obey the laws of ordinary algebra, e.g. AB - BA = 0 and AA^{-1} = 1

(b) Each operator is expressible in terms of the others.

Exercise D.2

Show that $\Delta = E\nabla$. Do this using the algebraic formulae and also on your spreadsheet. Similarly by algebra and the spreadsheet show that $E = 1 + \Delta$.
Remember that $1+\Delta$ is an *operator*. Thus, $[1+\Delta]\{f(m)\} = f(m)+\Delta\{f(m)\}$, not $1+\Delta\{f(m)\}$.

D.4 Inverse operators

From property (a) we know that $E^{-1}E = 1$. This means that $E^{-1}\{E\{f(m)\}\} = f(m)$. But, $E\{f(m)\} = f(m+1)$; therefore $E^{-1}\{f(m+1)\} = f(m)$.

Exercise D.3

1. Show that $\nabla = E^{-1}\Delta$.
   Again, do this using the algebraic formulae and also on your spreadsheet.
   Similarly show that $\nabla = 1 - E^{-1}$.
2. Note that you can do this with operator algebra if you use Exercise D.2 part 2, where we showed $E = 1 + \Delta$. Thus, $\Delta = E - 1$, and from part 1 of this exercise you have shown that $\nabla = E^{-1}\Delta = E^{-1}\{E - 1\} = 1 - E^{-1}$.
3. Hence justify the following table of relationships between the operators:

Operator	in terms of:		
	E	Δ	∇
E	E	$1+\Delta$	$(1-\nabla)^{-1}$
Δ	$E-1$	Δ	$\nabla(1-\nabla)^{-1}$
∇	$1-E^{-1}$	$\Delta(1+\Delta)^{-1}$	∇

D.5 Central differences

The central difference operator is usually used in *even* number orders of operation so that we do not need to know the value of our underlying function that are between our measured mesh points. For example:

$$
\begin{aligned}
\delta^2\{f(m)\} &= \delta\{\delta\{f(m)\}\} \\
&= \delta\{f(m+\frac{1}{2}) - f(m-\frac{1}{2})\} \\
&= \delta\{f(m+\frac{1}{2})\} - \delta\{f(m-\frac{1}{2})\} \\
&= [f(m+1) - f(m)] - [f(m) - f(m-1)] \\
&= f(m+1) - 2f(m) + f(m-1)
\end{aligned}
$$

Note we only have values at integer values of m again. This means that we can express δ^2 in terms of the other operators: $\delta^2 = \Delta\nabla$ or $= \nabla\Delta$.

For example:

$$\begin{aligned}
\delta^2\{f(m)\} &= \Delta\nabla\{f(m)\} \\
&= \Delta\{f(m) - f(m-1)\} \\
&= \Delta\{f(m)\} - \Delta\{f(m-1)\} \\
&= [f(m+1) - f(m)] - [f(m) - f(m-1)]
\end{aligned}$$

which is the same as before. Thus by use of *algebraic* formalism we can write $\delta = (\Delta\nabla)^{1/2}$. But, note that the *central difference* (and *averaging*) *operator* is usually applied twice. This will use values and yield results at the measured points, m.

It is useful to note the following relationships between the operators. As we will see, the implementation will partly be determined by convenience and partly by required accuracy.

$$\delta = E^{-1/2}\Delta = E^{1/2}\nabla = E^{1/2} - E^{-1/2} = \Delta(1+\Delta)^{-1/2} = \nabla(1-\nabla)^{-1/2} = 2(\mu^2 - 1)^{1/2}$$

$$\mu\delta = \frac{1}{2}(E - E^{-1}) = \frac{1}{2}(\Delta + \nabla)$$

$$E^{1/2} = \mu + \frac{1}{2}\delta$$

$$E^{-1/2} = \mu - \frac{1}{2}\delta$$

$$\mu = \frac{1}{2}(E^{1/2} + E^{-1/2}) = (1 + \frac{1}{2}\Delta)(1+\Delta)^{-1/2} = (1 - \frac{1}{2}\nabla)(1-\nabla)^{-1/2} = (1 + \frac{1}{4}\delta^2)^{1/2}$$

Next week we'll see what we can do with these operators, starting with interpolation.